SEARCH REQUEST FORM

Scientific and Technical Inf rmation Center

| Requester's Full Name: | BERCH | Examiner # | · O 59193 | Date: 7/2 | |
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| Please provide a detailed statement of | | | s possible the subje | ct matter to be se | arched. |
| Include the elected species or structure | s, keywords, synonyms, | acronyms, and regist | ry numbers, and cor | nbine with the co | oncept or |
| utility of the invention. Define any ter known. Please attach a copy of the cov | | | amples of relevant of | chations, authors | etc, ii |
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| Title of Invention: | | | • | | |
| Inventors (please provide full names |): | | | * | |
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| Earliest Priority Filing Date: | | | | | |
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     FILE 'REGISTRY' ENTERED AT 10:21:52 ON 09 JUL 2002
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L3
                E DIHYDROFOLATE/CN 5
                E THYMIDYLATE/CN 5
                E RTK/CN 5
                E RECEPTOR TYROSINE KINASE/CN 5
L4
              1 S E3
                E VEGF/CN 5
                E ANGIOGENESIS/CN 5
     FILE 'MEDLINE, HCAPLUS, EMBASE, JICST-EPLUS, BIOSIS' ENTERED AT 10:27:48
     ON 09 JUL 2002
L5
              O FILE MEDLINE
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              O FILE MEDLINE
L11
L12
             16 FILE HCAPLUS
              O FILE EMBASE
L13
              O FILE JICST-EPLUS
L14
              O FILE BIOSIS
L15
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(FILE 'CAOLD' ENTERED AT 10:21:19 ON 09 JUL 2002)

Searched by: Mary Hale 308-4258 CM-1 1E01

TOTAL FOR ALL FILES

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(oligonucleotide contg. in place of guanine, diagnosis or inhibition of
 nucleic acid function by triple helix formation with)
RN 150439-88-6 HCAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4,7-dihydro-4-(1-methylethylidene) (9CI) (CA INDEX NAME)

| L23 | 0 | FILE | MEDLINE |
|-----|----|------|-------------|
| L24 | 15 | FILE | HCAPLUS |
| L25 | 0 | FILE | EMBASE |
| L26 | 0 | FILE | JICST-EPLUS |
| L27 | 0 | FILE | BIOSIS |

TOTAL FOR ALL FILES L28 15 L16 NOT L22

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TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d 13 que stat;e dihydrofolate/cn 5
L1 STR

VAR G1=H/ME
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 1
CONNECT IS E2 RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L3 28 SEA FILE=REGISTRY SSS FUL L1

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E3
                 DIHYDROFOLATE DEHYDROGENASE/CN
E4
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                   DIHYDROFOLATE FORMYLTRANSFERASE/CN
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=> e thymidylate/cn 5
                   THYMIDINE-T/CN
E1
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                   ONIA SOLANACEARUM STRAIN GMI1000 GENE DEOA)/CN
             0 --> THYMIDYLATE/CN
                   THYMIDYLATE 5'-NUCLEOTIDASE/CN
E4
                   THYMIDYLATE 5'-PHOSPHATASE/CN
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             0 --> RTK/CN
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                   RTM 6/CN
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                   RTM 6 (EPOXY RESIN)/CN
=> e receptor tyrosine kinase/cn 5
                   RECEPTOR TYPE GUANYLYL CYCLASE (BOMBYX MORI CLONE BM-GC-I)/C
E2
                   RECEPTOR TYPE TYROSINE PHOSPHATASE H/CN
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             1 --> RECEPTOR TYROSINE KINASE/CN
E4
                   RECEPTOR TYROSINE KINASE (APLYSIA CALIFORNICA CLONE 2A/1A GE
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            1 "RECEPTOR TYROSINE KINASE"/CN
    ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
L4
RN
     340830-03-7 REGISTRY
CN
    Kinase (phosphorylating), receptor protein tyrosine (9CI) (CA INDEX NAME)
OTHER NAMES:
    Growth factor receptor kinase
CN
CN
     Growth factor-receptor tyrosine kinase
CN
     Receptor protein kinase
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     Receptor protein tyrosine kinase
CN
    Receptor tyrosine kinase
MF
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     STN Files: BIOSIS, CA, CAPLUS, TOXCENTER, USPATFULL
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
              90 REFERENCES IN FILE CA (1967 TO DATE)
              91 REFERENCES IN FILE CAPLUS (1967 TO DATE)
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Searched by: Mary Hale 308-4258 CM-1 1E01

1: 137:18792

REFERENCE

REFERENCE 2: 137:17453 REFERENCE 3: 137:15772 136:396038 REFERENCE 4 • 136:381016 REFERENCE 5: REFERENCE 6: 136:380176 136:380088 7: REFERENCE 136:365565 REFERENCE 8: REFERENCE 9: 136:363852 REFERENCE 10: 136:350606 => e vegf/cn 5 VEGETATIVE MYCELIUM HYDROPHOBIN 3 (PLEUROTUS OSTREATUS STRAI E1 N NOO1 GENE VMH3 PRECURSOR)/CN VEGETOX/CN E2 0 --> VEGF/CN E3 VEGF (CHICKEN)/CN E41 VEGF (HUMAN 148-AMINO ACID ISOFORM)/CN E5 => e angiogenesis/cn 5 ANGIOFILINE/CN 1 E1ANGIOFLEX/CN E2 1 0 --> ANGIOGENESIS/CN E3 ANGIOGENESIS ASSOCIATED PROTEIN HBAZF (HUMAN ORTHOLOG OF MOU E4 SE BAZF) (HUMAN)/CN ANGIOGENESIS ASSOCIATED PROTEIN HEF-G (HMT-ELONGATION FACTOR G) (HUMAN)/CN => fil medl, hcap, embase, jicst, biosis; s 13 and (14 or dihydrofol? or thymidyl? or rtk or receptor tyrosine kinase or 340830-03-7 or growth factor receptor kinase or growth factor receptor tyrosine kinase) SINCE FILE COST IN U.S. DOLLARS TOTAL. ENTRY SESSION 149.48 395.07 FULL ESTIMATED COST SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION -3.72CA SUBSCRIBER PRICE 0.00

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FILE 'BIOSIS' ENTERED AT 10:27:48 ON 09 JUL 2002

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O FILE MEDLINE
L5
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               GROWTH FACTOR RECEPTOR TYROSINE KINASE)
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             O FILE MEDLINE
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L22 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS
1993:575369 Document No. 119:175369 Formation of triple helix complexes of
     single stranded nucleic acids using oligonucleotides. Ts'O, Paul On Pong;
     Adams, Thomas Henry; Arnold, Lyle J., Jr. (Johns Hopkins University, USA;
     Genta Inc.). PCT Int. Appl. WO 9307295 Al 19930415, 98 pp. DESIGNATED
     STATES: W: AU, CA, FI, JP, KR, NO, RU; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE. (English). CODEN: PIXXD2. APPLICATION:
     WO 1992-US8458 19921005. PRIORITY: US 1991-772081 19911007.
     Triplex helix structure with a specific segment of single-stranded nucleic
AB
     acid can be formed with 1st and 2nd oligomers comprised of nucleosidyl
     units linked by internucleosidyl phosphorus linkages . The 1st oligomer
     is sufficiently complementary to the target segment to form duplex and the
     2nd oligomer has .gtoreq.7 nucleotidyl units that are sufficiently
     complementary to hybridize with the duplex to form triplex. Upon
     formation of the triple helix the nucleic acids of interest may be
     detected and its function or expression prevented. The 1st and 2nd
     oligomers may comprise an oligonucleotide, an alkyl- or
     aryl-phosphonothioate oligomer, or other analogs, e.g. methylphosphonate
     oligomers. They may also contain uncharged neutral oligomers and purine
     or pyrimidine analogs, e.g., 2'-O-Me-pseudoisocytidine, 6-Se-guanine, or
     6-isopropylidene-7-deaza-guanidine. One of applications of this method is
     to inhibit in vivo synthesis of a protein by targeting its mRNA, which can
     be used for treatment of diseases, e.g. viral infections and
     cancers.
TΤ
     150439-88-6
     RL: USES (Uses)
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16 S L3
L17
              O FILE MEDLINE
L18
              1 FILE HCAPLUS
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              O FILE EMBASE
L20
              O FILE JICST-EPLUS
L21
              O FILE BIOSIS
     TOTAL FOR ALL FILES
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L22
L23
              O FILE MEDLINE
             15 FILE HCAPLUS
L24
              O FILE EMBASE
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              O FILE JICST-EPLUS
              O FILE BIOSIS
L27
     TOTAL FOR ALL FILES
L28
             15 S L16 NOT L22
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L28 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2002 ACS

2002:159146 Document No. 136:369546 An Ab Initio Study of the Hydrogen Bond Energy of Base Pairs Formed between Substituted 9-Methylguanine Derivatives and 1-Methylcytosine. Kawahara, Shunichi; Uchimaru, Tadafumi; Taira, Kazunari; Sekine, Mitsuo (National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8565, Japan). Journal of Physical Chemistry A, 106(13), 3207-3212 (English) 2002. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

The substitution effect on hydrogen-bond energy of the Watson-Crick type base pair formation between 1-methylcytosine and chem. modified 9-methylguanine derivs. was evaluated by an ab initio MO theory. Introduction of an electron-withdrawing group on the 8-position or on the exo-cyclic amino moiety enforced the hydrogen bond. Neither the charge distribution nor the sepn. between the hydrogen bonding sites is found to be directly correlated with the strength of the hydrogen bonds.

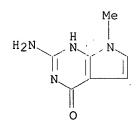
IT 90065-66-0 425428-05-3

RL: PRP (Properties)

(ab initio study of hydrogen bond energy of base pairs formed between substituted methylguanine derivs. and methylcytosine)

RN 90065-66-0 HCAPLUS

CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-amino-1,7-dihydro-7-methyl- (9CI) (CA INDEX NAME)



RN 425428-05-3 HCAPLUS

CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-amino-1,7-dihydro-7-methyl-, compd. with 4-amino-1-methyl-2(1H)-pyrimidinone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 90065-66-0 CMF C7 H8 N4 O

CM 2

CRN 1122-47-0 CMF C5 H7 N3 O

L28 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1996:499170 Document No. 125:221073 The synthesis and determination of acidic ionization constants of certain 5-substituted 2-aminopyrrolo[2,3-d]pyrimidin-4-ones and methylated analogs. Hoops, Geoffrey C.; Park, Julie; Garcia, George A.; Townsend, Leroy B. (Interdepartmental Grad. Program Med. Chem., Univ. Michigan, Ann Arbor, MI, 48109-1065, USA). J. Heterocycl. Chem., 33(3), 767-781 (English) 1996. CODEN: JHTCAD. ISSN: 0022-152X.

AB Acidic ionization consts. were detd. for a series of 5-substituted 2-aminopyrrolo[2,3-d]pyrimidin-4-ones and their N-3- and N-7-methylated analogs. The synthesis of the methylated analogs are also described.

IT 90065-66-0P 181480-33-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and detn. of acidic ionization consts. of aminopyrrolopyrimidinones)

RN 90065-66-0 HCAPLUS

CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-amino-1,7-dihydro-7-methyl- (9CI) (CF INDEX NAME)

RN 181480-33-1 HCAPLUS

CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-amino-1,7-dihydro-5,7-dimethyl- (9CI) (CA INDEX NAME)

IT 90065-71-7P 181480-32-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and detn. of acidic ionization consts. of aminopyrrolopyrimidinones)

RN 90065-71-7 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4-chloro-7-methyl- (9CI) (CA INDEX NAME)

RN 181480-32-0 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4-chloro-5,7-dimethyl- (9CI) (CA INDEX NAME)

L28 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1995:382828 Document No. 122:160677 Preparation of 4-(substituted alkyl amino)pyrrolo[2,3-d]pyrimidine derivatives for treatment and prevention of anoxia. Takenochi, Kazuya; Sakuma, Yasushi; Takeuchi, Takahiro; Furuya, Minoru; Kadota, Takashi; Horiuchi, Hideki; Yamanaka, Yoshihiro; Komorya, Keiji (Teijin Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 06329675 A2 19941129 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-118283 19930520.

GI

The title compds. (I; R1 = H, alkyl, alkenyl, aralkyl; R2 = alkyl, AΒ alkenyl, aralkyl; R3 = H, C1-3 alkyl; R4 = C1-6 alkylene; R5 = C2-6 alkylene, C6-10 arylene; R6 = H, C1-3 alkyl; A, B = O, S, NR, wherein R = H or C1-3 alkyl; when R5 = C2-6 alkylene, n = 1; when R5 = C6-10 arylene, n = 1-3) and pharmacol. acceptable salts are prepd. Thus, 5.00 q 2-amino-4-chloro-7H-pyrrolo[2,3-d]pyrimidine, 4.96 mL Et3N, and 10.08 q p-anisylchlorodiphenylmethane were stirred in DMF at room temp. for 30 min and cooled to 0.degree. followed by successively adding 4.50 mL MeI and 3.00 g NaH, reacting the resulting mixt. for 1 h, and successively adding $5.36\ \mathrm{mL}$ allyl iodide and $2.00\ \mathrm{g}$ NaH and the resulting mixt. was allowed to react for 1 h to give, after workup and silica gel chromatog., 53.1% 2-allylamino-4-chloro-7-methyl-7H-pyrrolo[2,3-d]pyrimidine (II). II 20.0, K2CO3 31.10, and LiI 15.6 g were added to a soln. of 33.6 g trans-4-(2-ethoxyethyl)cyclohexylamine in 60 mL BuOH in an autoclave and heated at 160.degree. and inner pressure 2-3 kgf/cm2 under N for 65 h to give, after workup and silica gel chromatog., 86% title compd. (III). III. H2SO4 was continuously administered at 0.1 mg/kg/min i.v. for 10 min to mice suffering anoxia in the state of breathing failure induced by injecting 2.0% aq. AcOH to the respiratory tract to show the increase in the partial pressure of O (PoO2) .DELTA.PoO2 = +13.7 mmHg, and the decrease in the partial pressure of CO2 in arterial blood (PoCO2) .DELTA.PoCO2 = -14.7 mmHg. Each tablet and injection formulation contg. III.H2SO4 were described.

Ι

II

IT 90065-71-7, 2-Amino-4-chloro-7-methyl-7H-pyrrolo[2,3-d]pyrimidine RL: RCT (Reactant)

(alkylation with Me iodide and allyl iodide in prepn. of (alkylamino)pyrrolopyrimidine derivs. for treatment and prevention of anoxia)

RN 90065-71-7 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4-chloro-7-methyl- (9CI) (CA INDEX NAME)

L28 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1994:508677 Document No. 121:108677 Trifluoromethylated pyrimidines starting from .beta.-trifluoroacetyl-lactams, -lactone and -cyclanone. Bouillon, Jean Philippe; Bouillon, Vincent; Wynants, Chantal; Janousek, Zdenek; Viehe, Heinz G. (Lab. Chim. Org., Louvain-la-Neuve, B-1348, Belg.). Heterocycles, 37(2), 915-32 (English) 1994. CODEN: HTCYAM. ISSN: 0385-5414. OTHER SOURCES: CASREACT 121:108677.

GI

AB A prepn. of trifluoromethylated pyrimidines from .beta.-trifluoroacetyl-lactams and -benzolactams is accomplished by reaction with benzamidine as bis(nucleophile). This condensation is also extended to cyclic trifluoromethylated 1,3-diketones and 3-aroyl-2-pyrrolidinones. Cyclocondensation of (trifluoroacetyl)lactams I (n = 0-2) gave the fused pyrimidines II (same n).

IT 156870-46-1P

RN 156870-46-1 HCAPLUS

CN 5H-Pyrrolo[2,3-d]pyrimidin-2-amine, 6,7-dihydro-7-methyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L28 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2002 ACS
1991:608603 Document No. 115:208603 Preparation of N-

[[(pyrrolopyrimidinyl)alkyl]benzoyl]glutamates and analogs as antitumor

antitumor

agents. Akimoto, Hiroshi; Ootsu, Koichiro (Takeda Chemical Industries, Ltd., Japan). Eur. Pat. Appl. EP 438261 A2 19910724, 34 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1991-300266 19910115. PRIORITY: JP 1990-7962 19900116.

GΙ

Title compds. [I; A = atoms to complete a 5-membered ring; R = ZBCONHCH(CO2R1)CH2CH2CO2R2; B = (un)substituted divalent cyclic or chain group (sic); R1, R2 = ester residue, cation; X = NH2, OH, SH; Y = H halo, (un)substituted OH, NH2, SH, hydrocarbyl; Z = (heteroatom-interrupted) (un)substituted (CH2)2-5; l of Z1, Z2 = N and the other = N or CH] were prepd. as antitumor agents (no data). Thus, pyrrolopyrimidine II (R = cyano) was heated 1.5 h at 75-80.degree. with Raney Ni in HCO2H and the product (II; R = CHO) was condensed with Ph3P+CH2C6H4(CO2Me)-4 Br- to give, after hydrogenation, II [R = CH2CH2C6H4(CO2Me)-4] which was sapond. and the product condensed with di-Et glutamate to give II [R = CH2CH2C6H4CONHCH(CO2Et)CH2CH2CO2Et].

IT 136784-81-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, in prepn. of antitumor agents)

RN 136784-81-1 HCAPLUS

CN Benzoic acid, 4-[3-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]- (9CI) (CA INDEX NAME)

IT 136784-19-5P 136784-20-8P 136784-23-1P 136784-46-8P 136784-47-9P 136784-48-0P 136784-49-1P 136784-56-0P 136784-58-2P

138262-39-2P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of, as antitumor agent)

RN 136784-19-5 HCAPLUS

CN L-Glutamic acid, N-[4-[2-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 136784-20-8 HCAPLUS

CN L-Glutamic acid, N-[4-[2-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} Me \\ H \\ N \\ N \\ N \\ \end{array}$$

RN 136784-23-1 HCAPLUS

CN L-Glutamic acid, N-[4-[3-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 136784-46-8 HCAPLUS

CN L-Glutamic acid, N-[4-[2-(2-amino-4,7-dihydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-6-yl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 136784-47-9 HCAPLUS

CN L-Glutamic acid, N-[4-[3-(2-amino-4,7-dihydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-6-yl)propyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 136784-48-0 HCAPLUS

CN L-Glutamic acid, N-[4-[2-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-6-yl)ethyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ H_2N & & & \\ N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 136784-49-1 HCAPLUS

CN L-Glutamic acid, N-[4-[3-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-6-yl)propyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 N
 N
 CO_2H
 N
 CO_2H

RN 136784-56-0 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2-amino-4,7-dihydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-6-yl)methyl]methylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 136784-58-2 HCAPLUS

CN L-Glutamic acid, N-[4-[[(2-amino-4,7-dihydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-6-yl)methyl]-2-propynylamino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 138262-39-2 HCAPLUS

CN L-Glutamic acid, N-[4-[3-(2-amino-4,5,6,7-tetrahydro-7-methyl-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 136784-96-8

RL: RCT (Reactant)

(reaction of, in prepn. of antitumor agents)

RN 136784-96-8 HCAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidine-6-methanaminium, 2-amino-4,7-dihydro-N,N,N,7-trimethyl-4-oxo-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 136784-95-7 CMF C11 H18 N5 O

$$\begin{array}{c|c} & \text{Me} \\ & \text{H}_2\text{N} \\ & \text{N} \\ & \text{O} \end{array}$$

CM 2

CRN 16053-58-0 CMF C H3 O3 S

L28 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2002 ACS
1987:614017 Document No. 107:214017 Dextran-linked 7-deazaguanine - a
polymer-bound inhibitor of xanthine oxidase. Rosemeyer, Helmut; Kaiser,
Klaus; Seela, Frank (Lab. Org. Bioorg. Chem., Univ. Osnabrueck,
Osnabrueck, D-4500, Fed. Rep. Ger.). Int. J. Biol. Macromol., 9(4),
205-10 (English) 1987. CODEN: IJBMDR. ISSN: 0141-8130.

AB Dextran-liked 7-deazaguanine as well as 7-deazahypoxanthine and allopurinol derivs. were prepd. by carbodiimide condensation of the 2-carboxyethyl intermediates with N-(6-aminohexyl)carbamoylmethylated dextran T80. The dextran-linked bases are degradable by endo-dextranase (EC 3.2.1.11) as demonstrated by time-dependent viscosity measurements.

Monomeric as well as polymer-linked purine analogs were tested as inhibitors of xanthine oxidase (EC 1.2.3.1) from cow's milk. Whereas the allopurinol- and 7-deazahypoxanthine derivs. no longer bind to the enzyme, the 7-deazaguanine derivs. are strong competitive inhibitors of xanthine oxidase even in the polymer-linked state.

IT 90065-66-0

RL: BIOL (Biological study)

(xanthine oxidase inhibition by, kinetics of)

RN 90065-66-0 HCAPLUS

CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-amino-1,7-dihydro-7-methyl- (9CI) (CA INDEX NAME)

L28 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1984:454781 Document No. 101:54781 Isomeric N-methyl-7-deazaguanines: synthesis, structural assignment, and inhibitory activity on xanthine oxidase. Seela, Frank; Bussmann, Werner; Goetze, Andreas; Rosemeyer, Helmut (Dep. Chem., Univ. Paderborn, Paderborn, D-4790, Fed. Rep. Ger.). J. Med. Chem., 27(8), 981-5 (English) 1984. CODEN: JMCMAR. ISSN: 0022-2623.

GΙ

The N-monomethyl isomers of 2-amino-3,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one (I) have been synthesized regiospecifically and their structures assigned. The 3-Me compd. was obtained by alkylation of I with Me2SO4, and the 1-Me isomer was obtained by condensation of (EtO)2CHCH2CH(CN)CO2Et with N-methylguanidine and subsequent cyclization. Methylation of 2-amino-4-chloro-7H-pyrrolo[2,3-d]pyrimidine, with MeI in the presence of 50% NaOH, by phase-transfer techniques, followed by the replacement of halide by hydroxyl, yielded the N7-Me compd. The N3-, N1-, and N7-Me isomers of I were all inhibitors of xanthine oxidase from cow milk with a Ki of 40, 3, and-4.5 .mu.M, resp.

IT 84955-33-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and ether cleavage of)

RN 84955-33-9 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4-methoxy-7-methyl- (9CI) (CA INDEX NAME)

IT 90065-74-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydrolysis of)

RN 90065-74-0 HCAPLUS

CN Ethanol, 2-[(2-amino-7-methyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)thio]- (9CI) (CA INDEX NAME)

IT 90065-71-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and methoxylation of)

RN 90065-71-7 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4-chloro-7-methyl- (9CI) (CA INDEX NAME)

IT 90065-66-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and xanthine oxidase-inhibiting activity of)

RN 90065-66-0 HCAPLUS

CN 4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-amino-1,7-dihydro-7-methyl- (9CI) (CA INDEX NAME)

L28 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1983:215558 Document No. 98:215558 Activated lactams: new syntheses of azacycloalka[2,3-d]pyrimidine and -[2,3-c]pyrazole derivatives. Takahata, Hiroki; Nakajima, Tomoko; Yamazaki, Takao (Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930-01, Japan). Synthesis (3), 226-8 (English) 1983. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 98:215558.

GI

AB Cyclization of enamines I (n = 1, 2) with amidines, RC(:NH)NH2, (R = NH2, Me, Ph) and hydrazines, R1NHNH2 (R1 = H, Ph), gave 53-71% II and 22-73% III, resp.

IT 85936-63-6P

RN 85936-63-6 HCAPLUS

CN 5H-Pyrrolo[2,3-d]pyrimidine-2,4-diamine, 6,7-dihydro-7-methyl-N4-phenyl-(9CI) (CA INDEX NAME)

L28 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1983:126554 Document No. 98:126554 Synthesis of acyclo-7-deazaguanosine by regiospecific phase-transfer alkylation of 2-amino-4-methoxy-7H-pyrrolo[2,3-d]pyrimidine. Seela, Frank; Kehne, Andreas; Winkeler, Heinz Dieter (Fachber. Naturwiss. II, Univ. Paderborn, Paderborn, D-4790, Fed. Rep. Ger.). Liebigs Ann. Chem. (1), 137-46 (German) 1983. CODEN: LACHDL. ISSN: 0170-2041. OTHER SOURCES: CASREACT 98:126554.

GΙ

Alkylating pyrrolopyrimidine I (R = H) with BrCH2O(CH2)2OAc in the presence of Bu4N+HSO4- gave 50% I [R = CH2O(CH2)2OAc], whose deacetylation gave 68% I [R = CH2O(CH2)2OH], which was treated with 4-MeSC6H4ONa in PhMe-(Me2N)3PO to give 69% acyclodeazoguanosine II.

IT 84955-33-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reactions of)

RN 84955-33-9 HCAPLUS

CN 7H-Pyrrolo[2,3-d]pyrimidin-2-amine, 4-methoxy-7-methyl- (9CI) (CA INDEX NAME)

L28 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1973:160087 Document No. 78:160087 Chemical studies on tuberactinomycin. V. Structures of guanidino amino acids in tuberactinomycins. Wakamiya, Tateaki; Shiba, Tetsuo; Kaneko, Takeo; Sakakibara, Hideo; Noda, Toshiharu; Take, Teruo (Fac. Sci., Osaka Univ., Toyonaka, Japan). Bull. Chem. Soc. Jap., 46(3), 949-54 (English) 1973. CODEN: BCSJA8.

GI For diagram(s), see printed CA Issue.

AB Tuberactinomycins A(I), B, N, and O, and component guanidino amino acids capreomycidine and tuberactidine (II) are discussed. The stereochem. of II was established. During isolation of II from a I hydrolyzate, it was converted to N.alpha.-formyltuberactidine dimer (III). In III alternation between a carbinolamine form of cyclol type and an amide lactone form depended on the pH. III was hydrolyzed to II and viomycidine with HBr. A pathway for the formation of viocidic acid, formed during hydrolysis of I, was proposed.

IT 19771-55-2P

CN 1H-1,3,5,7-Tetraazacyclopent[cd]indene-4-carboxylic acid, decahydro-6-imino-, dihydrobromide, [2aR-(2a.alpha.,4.beta.,4a.alpha.,7a.alpha.,7b.alpha.)]- (9CI) (CA INDEX NAME)

•2 HBr

L28 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1972:140698 Document No. 76:140698 Viomycin. I. Structure of the guanidine-containing unit. Bycroft, B. W.; Croft, L. R.; Johnson, A. W.; Webb, T. (Dep. Chem., Univ. Nottingham, Nottingham, Engl.). J. Chem. Soc., Perkin Trans. 1 (6), 820-7 (English) 1972. CODEN: JCPRB4.

GI For diagram(s), see printed CA Issue.

AB Viomycidin (I), obtained by acid hydrolysis of the Streptomyces antibiotic viomycin, is an artifact formed by cyclization of the monocyclic guanidinocarbinol unit (II). I gave capreomycidin (III) on hydrogenation and acid hydrolysis, and 2-aminopyridine on alk. hydrolysis, both products being derived from II.

RN 19771-55-2 HCAPLUS

CN 1H-1,3,5,7-Tetraazacyclopent[cd]indene-4-carboxylic acid, decahydro-6-imino-, dihydrobromide, [2aR-(2a.alpha.,4.beta.,4a.alpha.,7a.alpha.,7b.alpha.)]- (9CI) (CA INDEX NAME)

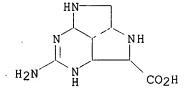
•2 HBr

RN 22265-96-9 HCAPLUS

CN 1H-1,3,5,7-Tetraazacyclopent[cd]indene-4-carboxylic acid, decahydro-6-imino-, [2dS-(2a.alpha.,4.alpha.,4a.beta.,7a.beta.,7b.beta.)]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 25990-48-1 CMF C8 H13 N5 O2



CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

RN 23250-09-1 HCAPLUS

CN 1H-1,3,5,7-Tetraazacyclopent[cd]indene-4-carboxylic acid, decahydro-6-imino-, dihydrochloride, [2aR-(2a.alpha.,4.beta.,4a.alpha.,7a.alpha.,7b.alpha.)]- (8CI, 9CI) /(CA INDEX NAME)

●2 HC1

L28 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2002 ACS
1971:411704 Document No. 75:11704 Structures of viocidic acid,
2-(2,3-dichloro-2-pyrrolin-1-yl)-1-pyrroline, and vicanicin. Suddath,
Fred L., Jr. (Georgia Inst. Technol., Atlanta, Ga., USA). 120 pp. Avail.
Univ. Microfilms, Ann Arbor, Mich., Order No. 70-17,969 From: Diss.
Abstr. Int. B 1970, 31(4), 1843-4 (English) 1970.

AB Unavailable

IT 25990-48-1

RL: PRP (Properties)
- (crystal structure of)

RN 25990-48-1 HCAPLUS

CN 1H-1,3,5,7-Tetraazacyclopent[cd] indene-4-carboxylic acid, decahydro-6-imino-, (2aS,4S,4aR,7aS,7bR)- (8CI, 9CI) (CA INDEX NAME)

L28 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2002/ACS

1970:449402 Document No. 73:49402 Structure and absolute configuration of viocidic acid: x-ray analysis of viocidic acid dihydrobromide. Coggon, Philip (Dep. of Chem., Duke Univ., Durham, N. C., USA). J. Chem. Soc. B (5), 838-45 (English) 1970. CODEN: JCSPAC.

The constitution and abs. stereochemistry of viocidic acid, a degradation product of viomycin, has been established by an x-ray crystal structure anal. of its dihydrobromide, C8H13N502.2HBr.3H2O. Crystals are orthorhombic, space group P212121, with Z = 4 in a unit cell of dimensions a 8.17, b 12.17, and c 15.22 .ANG... The at. coordinates were detd. by Fourier and least-squares calcns. and the final R value was 7.6% for 1408 independent reflections. The structure comprises dipos. C8H15N5O2 ions, bromide ions, and H2O mols.: H bonding is the dominant feature of the intermol. packing.

IT 28964-50-3

RL: PRP (Properties)
 (crystal structure of)

RN 28964-50-3 HCAPLUS

CN 1H-1,3,5,7-Tetraazacyclopent[cd]indene-4-carboxylic acid, decahydro-6-imino-, dihydrobromide, trihydrate, (2aS,4S,4aR,7aS,7bR)-(8CI) (CA INDEX NAME)

L28 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1969:106452 Document No. 70:106452 Structure, stereochemistry, and reactions of the guanidine moiety of viomycin. Bycroft, Barrie W.; Croft, L. R.; Johnson, Allen Woodward; Webb, Tesša (Univ. Nottingham, Nottingham, Engl.). J. Antibiot. (Tokyo), 22(3), 133-4 (English) 1969. CODEN: JANTAJ.

GI For diagram(s), see printed CA Issue.

AB Viomycin (I), contg. the unit A, was refluxed for 24 hrs. with 10N HCl; ion exchange chromatog. (Dowex 50 WX8) of the acid hydrolyzate yielded 2 basic amino acids, viomycidine (II), m. 200-4.degree., and viocidic acid

(III); dipicrate m. 173-5.degree.; dihydrochloride m. 210-12.degree.. gave a yellow ninhydrin reaction and a neg. Sakaguchi test. Based on the structure of III, abs. chirality was tentatively assigned for I and II at the .alpha. and .beta. centers. Catalytic redn. of I.HC1 with PtO2 in 3N HCl followed by acid hydrolysis gave no II, but yielded capreomycidine, m. 195.degree. (decompd.), [.alpha.]2D2.5 -22.7 (H2O), isolated as the free base. Mild base hydrolysis of I with 0.1N NaOH at 190 degree. for 20 hrs. followed by Et20 extn. yielded 2-aminopyrimidine (IV), m. 127-8.degree... Because II was not present in the total hydrolyzate of the resultant peptides, IV must have been obtained from the guanidine moiety. ΙT 22265-96-9P 23250-09-1P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 22265-96-9 HCAPLUS RN 1H-1, 3, 5, 7-Tetraazacyclopent[cd]indene-4-carboxylic acid, CN decahydro-6-imino-, [2aS-(2a.alpha.,4.alpha.,Aa.beta.,7a.beta.,7b.beta.)]-, compd. with 2,4,6-trinitrophenol (1:2) (9Cf) (CA INDEX NAME) CM 1 CRN 25990-48-1 CMF C8 H13 N5 O2 CDES * NΗ H₂N CO₂H CM 2 88-89-1 CRN C6 H3 N3 O7 CMF 02N NO2 OH NO₂ 23250-09-1 HCAPLUS RN 1H-1, 3, 5, 7-Tetraazacyclopent[cd]indene-4-carboxylic acid, CN decahydro-6-imino-, dihydrochloride, [2aR-(2a.alpha.,4.beta.,4a.alpha.,7a. alpha.,7b.alpha.)]- (8QI, 9CI) (CA INDEX NAME)

●2 HC1

L28 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2002 ACS

1968:487468 Document No. 69:87468 Viomycin. Further degradative studies.
Bycroft, B. W.; Cameron, D.; Croft, L. R.; Johnson, A. W.; Webb, Tessa;
Coggon, P. (Univ. Nottingham, Nottingham, Engl.). Tetrahedron Lett. (25),
2925-30 (English) 1968. CODEN: TELEAY.

GI For diagram(s), see printed CA Issue.

Mild hydrolysis of viomycin with 0.1N aq. NaOH gave 2-aminopyrimidine as well as a peptide mixt. (I). Chromatog. of I gave a cryst. dipeptide which was hydrolyzed to glycine and .alpha.,.beta.-diaminopropionic acid, indicating that the dipeptide is .alpha.,.beta.-diaminopropionylglycine. Acid hydrolysis of I gave glycine, .beta.-lysine, .alpha.,.beta.-diaminopropionic acid, and serine, indicating that viomycidine obtained from acid hydrolysis of viomycin is repleced by 2-aminopyrimidine and glycine in the alk. hydrolysis product. Hydrogenation of viomycin followed by total acid hydrolysis gave .alpha.-(2-iminohexahydro-4-pyrimidinyl)glycine. These results are explained by assuming the existence of the unit II in viomycin. Another degradation product, viocidic acid, was isolated as C8H13N5O2.2HBr.H2O and crystallized in the orthorhombic system group P212121, with 4 mols. per unit cell of dimensions a 8.17, b 12.17, and c 15.22 Å.

IT 19771-55-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 19771-55-2 HCAPLUS

CN 1H-1,3,5,7-Tetraazacyclopent[cd]indene-4-carboxylic acid, decahydro-6-imino-, dihydrobromide, (2aR-(2a.alpha.,4.beta.,4a.alpha.,7a.alpha.,7b.alpha.)]- (9CI) (CA INDEX/NAME)

●2 HBr

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L29 1 L3

=> d

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AN CA54:8840f CAOLD

TI possibility of evaluating the av. lifetime of the .alpha.-substructure within the nucleus

AU Serebrennikov, Yu. I.

TT 271-70-5 1421-27-8 1500-85-2 3680-69-1 3680-71-5 7355-55-7 7400-05-7 7400-06-8 7752-54-7 38897-11-9 39929-79-8 52133-67-2 52133-68-3 57564-92-8 60972-04-5 60972-05-6 60972-21-6 62981-81-1 63026-85-7 67831-83-8 67831-84-9 74895-37-7 74895-38-8 81965-21-1 90065-66-0 98198-24-4 98279-70-0 98279-99-3 98337-49-6 98337-52-1 98337-53-2 98338-15-9 98432-61-2 99584-71-1 99768-55-5 99975-97-0 99991-98-7 100047-45-8 100051-84-1 100137-44-8 100383-13-9 100396-59-6 100401-97-6 100453-73-4 102879-75-4 103648-99-3 108397-77-9 108630-80-4 108630-82-6 108748-93-2 108777-77-1 116154-69-9 116154-72-4 116154-73-5 120745-73-5

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